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Radiographic Spectroscopy of Atomic Composition of Materials: a Multi-Energy Approach

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A theoretical model of multi-energy radiography (MER) for reconstruction of the atomic structure is proposed. It is shown that, using multi-channel absorption and detection of radiation, effective atomic number and quantitative chemical composition of the materials can be readily reconstructed. This approach opens prospects for improvement of efficiency of X-ray techniques in non-destructive testing, nuclear and safety monitoring, security customs control, and others.

Digital (computer) radiography [1]-[3] is one of the new prominent methods in testing of materials. Its applications are often related to studies of the spatial structure of the inspected objects. Reconstruction of "geometrical" information is rather of qualitative character. Development of the technological base of modern non-destructive testing requires new methods allowing determination of specified properties of materials. Reconstruction of the "elemental" (atomic) composition of materials is one of the problems. Such monitoring is extremely important for control of the uranium content in active nuclear fuel elements or in nuclear waste drums [4]. It is necessary for inspection of loads or luggage with the aim of detection of explosives or other forbidden items [5]. Moreover, such reconstruction allows efficient separation of spatial images of complex and composed objects that are physically surimposed. In medicine, this leads to better distinction of soft and bone tissues [6]. Advantages of a technology combining inspection features for both spatial and atomic structure would be very significant.

Quantitative analysis of atomic/nuclear composition is generally related to the use of neutron methods. However, unlike radiography, these methods require sophisticated and expensive neutron spectroscopy equipment. It appears that there are no principal limitations for similar radiographic monitoring. This approach is based on the method of multi-energy radiography (MER). The multiplicity of radiography, i.e., number of required measurements carried at different energies of radiation, depends upon the number of quantitative characteristics of material composition that are subject to evaluation.

Among main physical parameters determining the chemical structure of a material, one should note the effective atomic number Z_{eff} and concentration $c_i = c(Z_i)$ of simple chemical elements with atomic number Z_i in a complex compound. Using a theoretical model of multi-energy radiography, in which all possible channels of partial absorption of the ionizing radiation in tested objects are accounted for, one can obtain theoretical expressions for these parameters. They can be reconstructed from radiographic data of MER. For a rough monitoring, two-energy radiography is sufficient. It allows reconstruction of the effective atomic number of the substance and the effective density of the tested sample (mass per unit area) of an for objects of unknown chemical composition. In a two-energy MER (see [1],[6]-[10] et al.), radiographic data are sampled by two detector systems that detect radiation in different ranges of the energy spectrum ($E_1 \neq E_2$). In the design, the efficient detectors for low-energy radiation (tens of keV) are scintillation detectors based on ZnSe(Te) crystals. For the medium-range energies (several hundreds of keV) the most suitable are CsI(Tl) crystals. Now substantial efforts are directed towards development of 3-radiography or high-multiplicity radiography, as well as the radiography using Compton back-scattering and the high-energy radiography in spectral region of the pair formation. The scheme of MER is shown in Fig. 1.

The MER allows also determination of the chemical composition of complex or multi-component substances. In the present work, we propose a new theoretical model of MER for reconstruction of the atomic/nuclear structure. Within the framework of the approach, we have obtained theoretical expressions for some main parameters of the structure of substances. These expressions depend only upon results of radiographic measurements and calibration (testing of objects of known composition and geometry). Therefore, they can be easily verified experimentally. The accuracy, priorities and prospects of the method are also discussed.

Determination of elemental concentrations c_i ($\sum c_i = 1$), i.e., of the relative content of simple elements in a complex compound or of the presence of admixtures, inclusions, etc. in a multi-component object, is the next step in development of MER methods. Solution of such problem makes it possible

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to efficiently distinguish between different single compounds in the structure of the tested object. As atomic numbers of these compounds are close to each other, their distinction is rather a difficult task. Without MER, it is hardly possible to get reliable information on chemical composition of the objects of monitoring. Among applications of such technique, we can note detection of explosives or other illegal substances or objects, environment monitoring, control of various solid-state or fluid media.

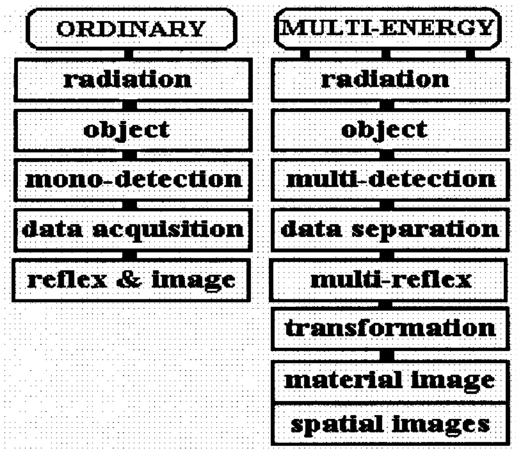

Fig. 1. Comparison of ordinary and multi-energy radiography.

Let us present resulting theoretical expressions for monitoring of atomic (chemical) structure of materials, which are useful for practical solution in the framework of two-energy radiography:

$$Z_{\text{eff}} = \left[\left(AR_1 + BR_2 \right) / \left(CR_1 + DR_2 \right) \right]^{1/p} . \quad (1)$$

$$c_i = c_i(R_1, R_2) = f_i(R_1, R_2) \times Z_i \left(Z_1 - Z_2 \right)^{-1} . \quad (2)$$

These formulas include only radiographic reflexes $R_i = \ln\left[V_0(E_i) / V_{\text{out}}(E_i) \right]$ (V_0 – is the background signal in the absence of objects; V_{out} – is the output detection signal; $i = 1,2$) and four calibration constants A, B, C, D corresponding the data of the measurements for samples of the known (but different) chemical composition and thickness. The degree $p = 3$ is for detection in the region of photo-effect, and $p = 1$ corresponds to the radiography with pair formation effect. Bulky expressions for $f_i = f_i(R_1, R_2; A, B, C, D)$ are not given explicitly. The concentrations c_i are determined for composition of two basic substances with known (reference) effective parameters Z_i ($Z_1 \neq Z_2$) in the tested object. Determination of Z_{eff} by formula (1) allows discerning between organic and inorganic compounds, e.g., organics hidden inside metal objects, cars, etc. Content of simple elements is controlled by determination of molar concentrations c_i from expression (2), ensuring distinction of certain organic substances against the background of other organic substances, e.g., explosives in plastic or paper envelopes, explosives mixed with sugar, etc.

In the new approach it is possible to limit oneself to the use of just the 2-radiography. This is important, because passing over to radiographies with higher multiplicity is a technically difficult task. To verify the theory, we compared the obtained theoretical dependence (1) with known experimental data on gamma-radiation absorption in a large range of various materials, starting from carbon ($Z = 6$) and ending with uranium ($Z = 92$). These results are shown in Fig. 2. In constructing the theoretical curves, three points were chosen as reference ones, defining a fraction-rational function in Eq. (1), which corresponded to materials with large, small and intermediate Z_{eff} values.

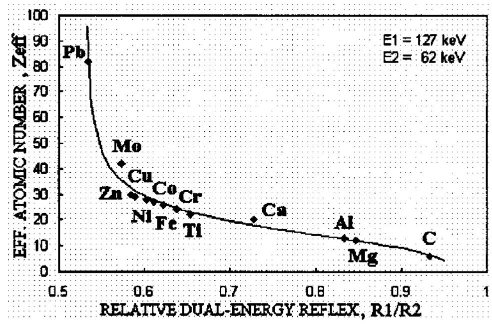

Fig. 2. Effective atomic number vs. 2-energy radiography reflexes.

The data presented are in a good agreement with theory.

Thus, our principal conclusion is that MER is just the method that is the well suitable for quantitative remote monitoring of the chemical composition of materials. Moreover, MER, unlike conventional techniques, allows more precise determination of spatial structure in complex, multi-component and multi-layered objects. Especially simple is 2-radiography. For more precise identification, 3- and 4-radiography should be used. The multi-energy method is suitable for determination of the chemical formula of an arbitrary material, as well as discerning of images obtained for objects with any number of "layers". Various modifications of MER can form a base for new development of non-destructive testing.

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